Energy levels of the configurations $4s^2 4p$, $4s4p^2$, $4s^2 4d$, and $4s^2 5p$ in Kr VI, obtained from a θ-pinch light source

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The spectrum of Kr VI has been observed in the 450–1000-Å wavelength range, and 15 lines have been identified as transitions between levels of the $4s^2 4p$, $4s4p^2$, $4s^2 4d$, and $4s^2 5p$ configurations. For seven of the lines the classification is new. All but three of the 14 levels that belong to the configurations have been determined. The result of this analysis is supported by isoelectronic comparisons along the Ga I isoelectronic sequence. The configurations are interpreted by fitting the theoretical energy parameters to the observed levels with use of least-squares techniques.

I. INTRODUCTION

Kr VI belongs to the Ga I isolelectronic sequence. Ions in this isoelectronic sequence have the ground configuration $4s^2 4p$ with the term ^2P.

The present work concerns the study of the configuration $4s^2 4p$ and the excited configurations $4s4p^2$, $4s^2 4d$, and $4s^2 5p$. Transitions to the ground configuration from these excited configurations have been observed in the ions Ga I–Br V and the results are presented in Ref. 1. For Br V Budhiraja and Joshi[2] revised and extended the results previously known. For Kr VI Fawcett *et al.*[3] reported eight lines as combinations from $4s4p^2$ and $4s^2 4d$ configurations to the $4s^2 4p$ ground configuration. For more highly ionized ions the $4s^2 4p-4s4p^2$ transitions of galliumlike ions from Rb VII to In XIX were observed by Reader *et al.*[4]

Curtis *et al.*[5] have observed the $4s^2 4p$ ^2P intervals in the Ga isoelectronic sequence from Rb VII to In XIX. More recently, Curtis[6] has predicted the fine-structure intervals for the lowest ^2P term in the Ga I isoelectronic sequence for $Z \leq 92$.

The revival of interest in spectroscopic data from rare gases is due to applications in collision physics, laser physics, photoelectron spectroscopy, and fusion diagnostics. In this last field the study of forbidden transitions (magnetic dipole transitions, $M1$) between low-lying fine-structure levels in highly ionized ions for systems with ground-state electron configuration of the form ns^2np produces strong line radiation and this is a very useful diagnostic tool for the analysis of high-temperature astrophysical and laboratory plasma.[7–10]

The spectra of Kr VI have been studied before using the beam-foil technique[11–13] and a capillary light source.[14]

II. EXPERIMENT

The experiments were performed with a θ-pinch discharge built at Lund Institute of Technology.[15] The θ-pinch device has a total capacitance of 7.7 μF and total inductance 76 nH. The maximum current at 10 kV discharge voltage is about 100 kA. The repetition rate of the discharge is about 15 per minute at a capacitor bank voltage of 10 kV.

The tube of the θ-pinch was connected to the spectrograph through metal bellows because our experiments were realized in the vacuum region. The spectra were recorded using a 3-m normal-incidence spectrograph equipped with a 1200–lines/mm grating blazed for 1380 Å. The plate factor in the first diffraction order is 2.77 Å mm^{-1}.

The spectra were exposed on Kodak SWR emulsion plates, and lines from Kr II–Kr VII were observed besides impurity lines from a low degree of ionization, which were used as internal standards. To distinguish between different stages of ionization, a number of experimental parameters, i.e., gas pressure in the tube, discharge voltage, and the number of discharges, were varied. A good spectrum of Kr VI was obtained with the following parameters: 5 mTorr, 13 kV, and 600 discharges. Plates were measured with a Zeiss Abbe compared with a photoelectric setting device.[16] This method of measurement allows us to detect asymmetric lines, since the line contours are displayed on an oscilloscope screen. For sharp lines the settings are reproducible to within ± 0.5 μm. A third-order interpolation formula was used to reduce the comparator settings to wavelength values. Our estimated wavelength uncertainty is ± 0.01 Å.

III. WAVELENGTHS AND ENERGY LEVELS

The wavelengths, intensities, and classification of the Kr VI lines are given in Table I. The intensities of the lines are based on visual estimates. Fifteen lines have been identified, at which seven are without previous classification.

TABLE I. Identified lines of Kr VI.

Intensity	Wavelength (Å)	Wave number (cm^{-1}) Observed	Calculated	Transition
8	450.20[a]	222 123.5	6.5	$4s^24p\ ^2P_{1/2}-4s^24d\ ^2D_{3/2}$
9	465.27[a]	214 929.0		$4s^24p\ ^2P_{3/2}-4s^24d\ ^2D_{5/2}$
6	467.25	214 018.2	5.2	$4s^24p\ ^2P_{3/2}-4s^24d\ ^2D_{3/2}$
6	544.02[a]	183 816.8		$4s^24p\ ^2P_{1/2}-4s^24p\ ^2P_{3/2}$
8	554.51[a]	180 339.4		$4s^24p\ ^2P_{1/2}-4s^24p\ ^2P_{1/2}$
9	569.13[a]	175 706.8	5.5	$4s^24p\ ^2P_{3/2}-4s^24p\ ^2P_{3/2}$
6	580.63[a]	172 226.7	8.1	$4s^24p\ ^2P_{3/2}-4s^24p\ ^2P_{1/2}$
4	595.97	167 793.7	6.6	$4s^24p\ ^2P_{1/2}-4s^24p\ ^2S_{1/2}$
7	626.22	159 688.3	5.3	$4s^24p\ ^2P_{3/2}-4s^24p\ ^2S_{1/2}$
8	705.85[a]	141 673.2	4.6	$4s^24p\ ^2P_{1/2}-4s^24p\ ^2D_{3/2}$
9	742.83[a]	134 620.3		$4s^24p\ ^2P_{3/2}-4s^24p\ ^2D_{5/2}$
5	748.70	133 564.8	3.3	$4s^24p\ ^2P_{3/2}-4s^24p\ ^2D_{3/2}$
2	935.97	106 841.0	0.7	$4s^24d\ ^2D_{3/2}-4s^25p\ ^2P_{3/2}$
9	944.05	105 926.6		$4s^24d\ ^2D_{5/2}-4s^25p\ ^2P_{3/2}$
4	956.03	104 599.2		$4s^24d\ ^2D_{3/2}-4s^25p\ ^2P_{1/2}$

[a]Previously identified by Fawcett *et al.* (Ref. 3).

The energy levels derived from the observed lines are given in Table II. The new lines of 935.97, 944.05, and 956.03 Å allow us to combine the $4s^24d$ and $4s^25p$ configurations and determine the level structure of the $4s^25p$ configuration. The 595.97- and 626.22-Å new lines determine the new level $4s^4p^2\ ^2S_{1/2}$.

When performing the analysis of the spectra we used isoelectronic extrapolation[17] along the Ga sequence, from Ga I up to Kr VI. The results of this extrapolation are shown in Fig. 1. In this figure the level $4s^24p\ ^2P_{3/2}$ was taken as a reference point and its energy value is set to zero; Z is the charge of the core, for example, $Z=6$ for Kr VI; and 1.8 is a constant empirically determined. In Fig. 2 we can see the gross structure of the lowest part of the Kr VI energy-level system.

In the analysis of the energy levels we also used theoretical predictions of the structure of the configurations. The predictions were obtained by diagonalizing the energy matrices with appropriate Hartree-Fock[18] (HF) values for the energy parameters. For this purpose the computer code developed by Cowan[19,20] was used. All but three of the 14 energy levels of the four configurations were determined.

IV. THEORETICAL INTERPRETATION

The configuration level structures were theoretically interpreted by a least-squares fit of the observed levels. In Table II we give, in addition to the observed level values, the differences between observed level values and those obtained from the fitted parameters. We also give in this table the percentage eigenvector composition.

In the calculation for the even-parity configurations, i.e., $4s4p^2$ and $4s^24d$, a configuration-interaction parameter was included, because there is a strong interaction between those configurations. The Hartree-Fock value for the configuration integral is 77 526 cm^{-1}. There are strong interactions between the levels $4s4p^2\ ^2D_{3/2}$ and $4s^24d\ ^2D_{3/2}$, and between $4s4p^2\ ^2D_{5/2}$ and $4s^24d\ ^2D_{5/2}$. Those interactions mixed the levels belonging to the two configurations and we can see this mixture in the percen-

TABLE II. Energy levels of Kr VI.

Designation	Energy (cm^{-1})	Obs.-Calc. (cm^{-1})	Percentage[a] composition
$4s^24p\ 2P_{1/2}$	0.0		100
$4s^24p\ 2P_{3/2}$	8111.3		100
$4s4p^2\ 2D_{3/2}$	141 674.6	−22	86 $(4s4p^2\ ^2D)$+13 $(4s^24d\ ^2D)$
$4s4p^2\ 2D_{5/2}$	142 731.6	20	86 $(4s4p^2\ ^2D)$+13 $(4s^24d\ ^2D)$
$4s4p^2\ 2S_{1/2}$	167 796.6		94 (^2S)+5 (^2P)
$4s4p^2\ 2P_{1/2}$	180.339.4	16	94 (^2P)+5 (^2S)
$4s4p^2\ 2P_{3/2}$	183 816.8	−14	98
$4s^24d\ 2D_{3/2}$	222 126.5	4	86 $(4s^24d\ ^2D)$+13 $(4s4p^2\ ^2D)$
$4s^24d\ 2D_{5/2}$	223 040.3	−3	86 $(4s^24d\ ^2D)$+13 $(4s4p^2\ ^2D)$
$4s^25p\ 2P_{1/2}$	326 725.7	−9	100
$4s^25p\ 2P_{3/2}$	328 967.2	8	100

[a]Percentages lower than 5% are omitted. The average LS purities of the $4s^24p$ and $4s^25p$ configurations are 100%; for $4s4p^2$ and $4s^24d$ configurations, 86%.

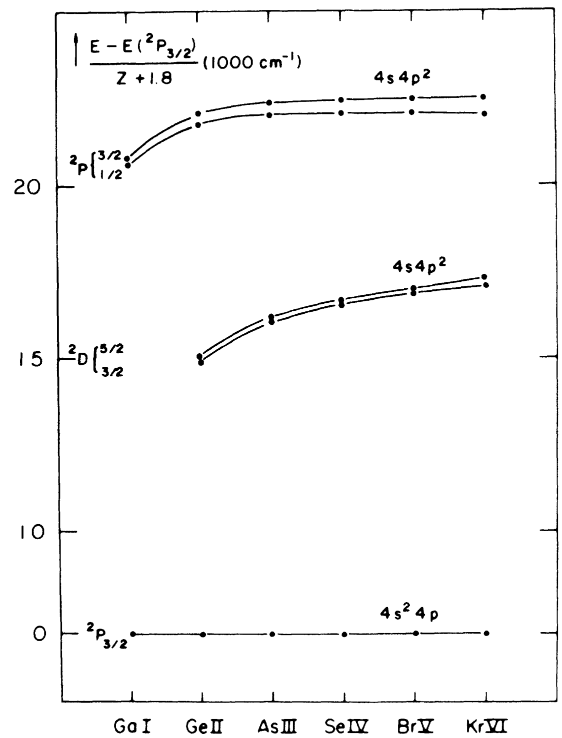

FIG. 1. Isoelectronic comparison of the $4s4p^2$ levels. The energy of the $4s^24p\ ^2P_{3/2}$ level is set to zero.

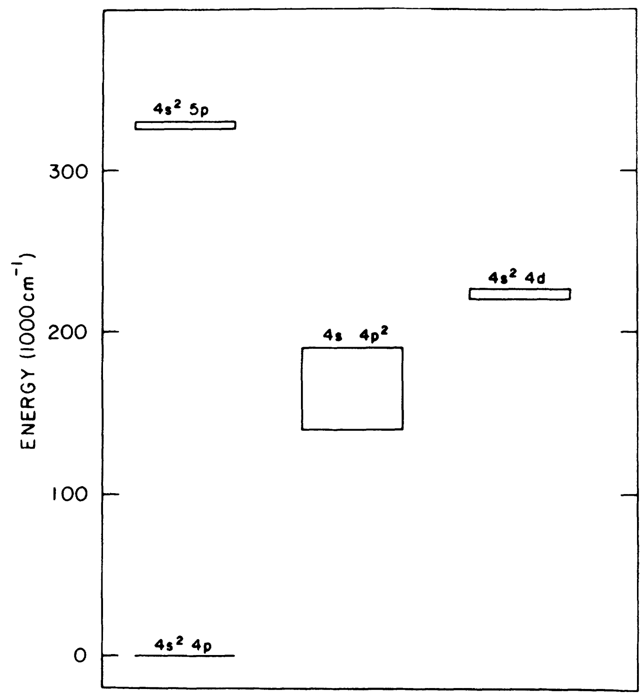

FIG. 2. Block diagram of the lowest configurations of Kr VI. There are two levels in $4s^24p$, ten levels in $4s4p^2$, two levels in $4s^24d$, and two levels in $4s^25p$.

TABLE III. Energy parameters for the $4s^24p$ and $4s^25p$ configurations of Kr VI.

Configuration	Parameter	HF value (cm^{-1})	Fitted value[a] (cm^{-1})	Fit/HF
$4s^24p$	E_{av}	0.0	5408	
	ζ_{4p}	4836	5408	1.118
$4s^25p$	E_{av}	317 269	328 217	1.034
	ζ_{5p}	1483 (fix)		

[a]The rms deviation of the fit is 12 cm^{-1} for four out of four observed levels.

TABLE IV. Energy parameters for the $4s4p^2$ and $4s^24d$ configurations of Kr VI.

Configuration	Parameter	HF value (cm^{-1})	Fitted value[a] (cm^{-1})	Fit/HF
$4s4p^2$	E_{av}	137 507.0	150 783.0	1.096
	$F^2(4p,4p)$	67 566.0	33 189.0	0.491
	$\alpha(4p,4p)$		−470.0 (fix)	
	$G^1(4s,4p)$	90 160.0	52 230.0	0.579
	ζ_{4p}	4183.0	4386.0	1.048
$4s^24d$	E_{av}	208 167.0	211 072.0	1.014
	ζ_{4d}	335.0	439.0	1.310
Configuration-interaction integral $4s4p^2$-$4s^24d$	$R^1(4p4p,4s4d)$	77 526.0 (fix)		

[a]The rms deviation of the fit is 37 cm^{-1} for seven out of ten observed levels.

tage eigenvector composition in Table II.

The integral $R^1(4p4p,4s4d)$ for the interaction configuration was kept fixed in the calculation. This reduced the mean error of the least-squares fit from 459 to 174 cm^{-1}.

In addition to the Slater, spin-orbit, and configuration-interaction parameters, we have included an effective electrostatic parameter $\alpha(4p,4p)$ (refs. 21–23) belonging to the configuration $4s4p^2$. The value of the α parameter is a fitted one and it is fixed in the calculation. The introduction of the α parameter lowered the rms deviation from 174 to 37 cm^{-1}.

The values of the parameters for the odd configurations $4s^24p$ and $4s^25p$ are in Table III. For the even configurations $4s4p^2$ and $4s^24d$ and results are in Table IV.

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